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9. PERFORMING ORGANIZATION NAME AND ADDRESS:
University of Miami
Department of Physics
Coral Gables, Florida 33124

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19. KEY WORDS (Continue on reverse side if necessary and identify by block number)

Detonation Failure

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

Qualitative results are obtained for detonation failure due to expansion losses. The equations for the Mach number and the reaction progress variable are integrated approximately. For certain loss ranges two detonation speeds are obtained. The slow one is actually the deflagration root that evolves beyond Mach one. For larger losses detonation failure occurs.

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AFOSR-TR- 82-0182

FINAL SCIENTIFIC REPORT

AIR FORCE OFFICE OF SCIENTIFIC RESEARCH

MINIGRANT NUMBER AFOSR80-0135

'Analytical Studies of Non-Ideal explosives'

Principal Investigator: Dr. Manuel A. Huerta
Department of Physics
University of Miami
Coral Gables, Florida 33124

ABSTRACT

Qualitative results are obtained for detonation failure due to expansion losses. The equations for the Mach number and the reaction progress variable are integrated approximately. For certain loss ranges two detonation speeds are obtained. The slow one is actually the deflagration root that evolves beyond Mach one. For larger losses detonation failure occurs.

SUMMARY OF RESEARCH RESULTS

To avoid repetition, the initial proposal is attached at the end as a part of this Final Report. The basic equations are Eqs.(47),(40), and (46) of the proposal,

$$\frac{2(1-m)dm/dz}{m(1+\gamma m)(2+(\gamma-1)m)} = \frac{d(\sum_i \lambda_i q_i)/dz}{\sum_i \lambda_i q_i + H_1 + u_1{}^2/2} - \frac{2\varepsilon}{(1+\gamma m)} \tag{47}$$

where $\varepsilon=(1/A)dA/dz$,

$$d\lambda_i/dz = R_i/u \quad , \tag{40}$$

and

$$c^2=\gamma p/\rho= \frac{2(\gamma-1)}{2+(\gamma-1)m}(\sum_i \lambda_i q_i + H_1 + u_1{}^2/2) \quad . \tag{46}$$

The crucial point is that the right hand side of eq.(47) has to be zero at the sonic point where the Mach number squared, $M^2=m=1$. This condition, in conjunction with Eq.(40) will determine the value of m right behind the initiating shock at z=0. We call this $m(z=0)=m_1=(u_1/c_1)^2$.

The above equations have been studied for realistic reaction rates and for different expansion losses. The work of Tsuge[1], Wecken[2], and others, summarized by Fickett and Davis[3], has been purely numerical. They have used a shooting method to find m_1, which enters the calculation as a kind of eigenvalue. They found that there are two

detonation velocities. One increases and the other one decreases as the expansion loss increases. At a critical loss the two roots coincide. Beyond this the two roots vanish indicating that there is no steady detonation solution. This is detonation failure.

In this work to understand detonation failure qualitatively, I began by studying the phase plane of Eqs.(40) and (47). The phase plane is extraordinarily complex. The phase orbit begins at the point $z=\lambda=0$ where $m=m_1$ and, with m_1 to be determined in such a way that the orbit reaches the $m=1$ line with a finite slope $dm/d\lambda$. This can occur only at the intersections of the curves $dm/d\lambda=0$ and $m=1$. The curve $dm/d\lambda=0$ is not very complicated qualitatively, even in the cases where one takes realistic temperature dependent reaction rates. The problem is that the curve contains m_1 as a parameter. For different values in the physical range $(\gamma-1)/2\gamma<m_1\leq 1$, the curves look radically different; even the number of critical points changes as one varies m_1. By this method it was not clear how to go beyond the results in Ref.3 and categorize the behavior of m_1 (and therefore D) as a function of the loss parameter ε. The approach discussed below bore much more fruit.

It turns out that Eq.(47) can be integrated very simply. The integrated equation evaluated at the sonic point $z=z_s$, $m=1, \lambda=\lambda_s$, and $c=c_s$, yields an exact equation for m_1,

$$\frac{(1+\gamma m_1)^2}{(1+\gamma)m_1} = (2+(\gamma-1)+2(\gamma-1)\sum_i \lambda_i q_i/c_1^{\,2})\Delta \tag{1f}$$

where $$\Delta = \exp-\int_0^z \frac{2\varepsilon}{(1+\gamma m)}\,dz \quad .$$

To get the form of Eq.(1f), Eq.(46) evaluated at $z=0$ has been used. The quantities behind the shock are related to those in front by the usual Hugoniot relations

$$m_1=M_1^2=\frac{2+(\gamma-1)m_0}{2\gamma m_0-(\gamma-1)}$$

and

$$c_1^2=c_0^2=\frac{(2\gamma m_0-(\gamma-1))(2+(\gamma-1)m_0)}{(\gamma+1)^2 m_0}$$

in accordance with Eq.(15). Here $m_0=M_0^2$ is the Mach number squared in the unreacted explosive in front of the shock and c_0 is the speed of sound there. The detonation velocity D is given by $D^2=m_0c_0^2$. When we substitute for m_1 and c_1 in Eq.(1f) in terms of m_0 and c_0, we obtain

$$\frac{(1+\gamma m_0)^2}{(1+\gamma)m_0}=(2+(\gamma-1)m_0+2(\gamma-1)\sum_i\lambda_{is}q_i/c_0^2)\Delta \qquad (2f)$$

It may seem strange that Eq.(2f) has the same form as Eq.(1f). This should not surprise us, however, because the conservation equations are integrated across the shock front via the Hugoniot relations for $m_0>1$, whereas we simply put $m_1=m_0$ for $m_0<1$. The features of Eq.(2f) can be understood qualitatively. The value of m_0 is found from the intersections of the graphs of the left and right sides of Eq.(2f) versus m_0, keeping in sight the m_0 dependence of $\Delta(\varepsilon,m_0)$. For the case $\varepsilon=0$, $\lambda_{is}=1$, $\Delta(0,m_0)=1$, we obtain Fig.1. The two roots m_{0-} and m_{0+} are found. m_{0-} represents a no-shock Chapman-Jouguet

deflagraion. m_{0+} is the Chapman-Jouguet detonation solution. As ε increases, $\Delta(\varepsilon,m_0)$ decreases. In the proposal the dependence of Δ on m_0 was ignored. Then, as ε increases, the straight line for $\varepsilon=0$ is simply brought down with a reduced slope until the two roots meet at some value $m<1$ and then disappear below Mach one. The comments in the proposal regarding Tsuge's results were not really valid, then, because he considered temperature dependent reaction rates in his numerical calculations. The temperature dependence changes things because it has an important effect on the m_0 dependence of $\Delta(\varepsilon,m_0)$. This effect can be understood approximately by studying $\Delta(\varepsilon,m_0)$ for a simple case.

Let us take ε = constant so it can be brought out of the integral. This is the case considered by Wecken[2] (actually, one has to solve for the expansion as a free boundary problem of great complexity). The term $1 + \gamma m$ in Δ is a smooth, well behaved function of z. It increases pretty much linearly from its value $1 + \gamma m_1$ at $z=0$ to its value $1 + \gamma$ at $z=z_s$ as can be seen by examining the results in page 51 of Ref.3. This linear behavior is in marked contrast to the z dependence of u, c, p, T, λ, and other relevant quantities, which exhibit a characteristic step-like behavior. Putting $m=1$ in the integral for Δ will not affect the problem very much. In fact, putting $m=1$ minimizes the loss effect of Δ. Therefore we will just take

$$\Delta = \exp-\left(\frac{2\varepsilon z_s}{1 + \gamma}\right) \qquad (3f)$$

The strong m_0 dependence of Δ, due to the temperature dependent reaction rate, is hidden in z_s. To show this let us take

$$d\lambda/dz = k\ (1 - \lambda)^2\ \exp(-T_a/T)\ ,$$

where k is a constant, for Eq.(40). This is not an entirely realistic reaction rate because k should be a function of T and m. The T dependence with the strongest effect on the solution is contained in the exponential, however. We write T as

$$T = (M_w/R)p/\rho = (M_w/R)c^2/\gamma\ ,$$

or

$$T = (M_w/R)\ \frac{2(\gamma-1)q(\lambda+h)}{2 + (\gamma-1)m}$$

where M_w is the molecular weight of the gas, R is the universal gas constant, and

$$h = (\ H_1 + u_1{}^2/2)/q = \frac{c_0{}^2(\ 2 + (\gamma-1)m_0)}{q(\gamma-1)}\ .$$

In the cases where $c_0{}^2 \ll q$ we can have $h \ll 1$ if m_0 is near one as in a weak detonation. If m_0 is large, however, h is close to γ^2-1 (γ=3 is a good value). Since $0 \leq \lambda \leq 1$ and $m_1 \leq m \leq 1$, the strong detonation behavior is well represented even if we neglect the spatial variation in T. Therefore we take

$$T = (M_w/R)\,\frac{4(\gamma-1)q(1+h)}{(\gamma+1)^2} \quad .$$

where the minimum value $\gamma-1/2\gamma$ has been used for m in the denominator. This overestimate for T makes the reaction rate as large as it can be thereby minimizing the loss effect due to Δ. The reaction equation is

$$d\lambda/dz = r(1-\lambda)^2 \quad . \tag{4f}$$

with

$$r = k\,\exp-(b/(1+h)) \quad .$$

The above expression can be handled easily and has the virtue that it preserves the m_w dependence via h. Integrating Eq.(4f) with the boundary conditions $\lambda=0$ at $z=0$, and $\lambda=\lambda_s$ at $z=z_s$, we get

$$1-\lambda_s = 1/(1+rz_s) \quad .$$

Going back to Eq.(47), we impose the condition that the right hand side is zero at $\lambda=\lambda_s$, $z=z_s$, $m=1$,

$$\frac{r(1-\lambda_s)^2}{\lambda_s+h} = \frac{2\varepsilon}{1+\gamma} \quad . \tag{5f}$$

Solving for λ_s we get

$$\lambda_s = 1 - \frac{2(1+h)}{1+\left[1+4(1+\gamma)(1+h)r/2\varepsilon\right]^{1/2}} \tag{6f}$$

and then

$$z_s = \lambda_s / r(1-\lambda) \quad . \tag{7f}$$

The expression above allows $\lambda_s < 0$ when $h > r(1+\gamma)/2\varepsilon$. This is not allowed and it indicates where Eq.(5f) cannot be satisfied. When Eqs.(6f) and (7f) are substituted into Eqs.(2f) and (3f) one should not take seriously the portions where $\lambda_s < 0$. A plot of Eq.(2f) is given in Fig.2 for $\varepsilon=0.005$. In Fig.2 the right hand side has been made zero wherever $\lambda_s < 0$. The two roots $m_{0-}=2.74$ and $m_{0+}=10.3$ are found.
For this example we have taken the parameters of Ref.3, page 46 (except for b which is taken smaller). With these values the solutions are well into the double detonation range. A natural dimensionless loss parameter δ is defined by

$$\delta=(\varepsilon/k)^{1/2}.$$

A numerical procedure was used to find the roots, being careful about the $\lambda_s < 0$ problem. The results are presented in the Table below. The speed of sound in the unreacted material is taken to be $c_0=1367$ m/sec. as in Ref.3. The roots at $\delta=0$ in the Table are the ideal CJ deflagration and detonation roots. For δ less than about 0.0025 there are still a deflagration and a detonation root. A little above that value the deflagration root goes above Mach one to become a slow detonation root. The fast detonation root decreases while the slow detonation root increases with δ. Near the value $\delta=.00715$ the two detonation speeds become equal and then disappear. For $\delta=.0072$, there are no roots. Detonation failure has taken place. The variation of the slow root is very fast for small values of δ. This is probably the reason why Tsuge could not

follow the slow root in his numerical calculations. The values in the Table are plotted in Fig.3. The curve is very similar to those obtained in the numerical calculations discussed in Ref.3. Clearly, as the diameter loss parameter δ is reduced, the slow detonation root goes to Mach one as conjectured by Tsuge[1].

The above results are based on an approximation that overestimates the reaction rate by overestimating T. This gives a lower bound for Δ. Further work is needed to find an upper bound for it and thus bound it from both sides.

TABLE I

δ	m_{0-}	m_{0+}	Dslow(m/s)	Dfast(m/s)
0.0	0.047	21.47	294.78	6334.10
0.000001	0.052	21.31	311.72	6310.45
0.00001	0.067	20.90	353.84	6249.45
0.00005	0.10	20.30	434.44	6159.10
0.0001	0.14	19.86	502.27	6091.98
0.0002	0.19	19.20	599.00	5890.00
0.0003	0.25	18.70	676.63	5911.39
0.0004	0.30	18.30	742.47	5847.82
0.0005	0.34	18.0	797.09	5799.69
0.0008	0.46	17.0	927.14	5636.29
0.001	0.54	16.52	1004.54	5556.14
0.002	0.86	14.50	1268.44	5205.38
0.0025	0.99	13.70	1360.15	5059.75
0.0030	1.35	12.97	1588.31	4923.10
0.0035	1.71	12.3	1787.58	4794.25
0.0040	2.04	11.6	1952.47	4655.83
0.0044	2.31	11.1	2077.66	4554.39
0.005	2.74	10.3	2262.79	4367.20
0.006	3.60	8.8	2593.70	4055.18
0.007	5.10	6.9	3087.12	3590.82
0.0071	5.40	6.5	3176.62	3485.18
0.00715	5.88	6.0	3314.80	3351.24
0.72	no root	no root	no root	no root

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3. Fickett, W. and Davis, W.C., Detonation. Berkeley: University of California Press. 1979.

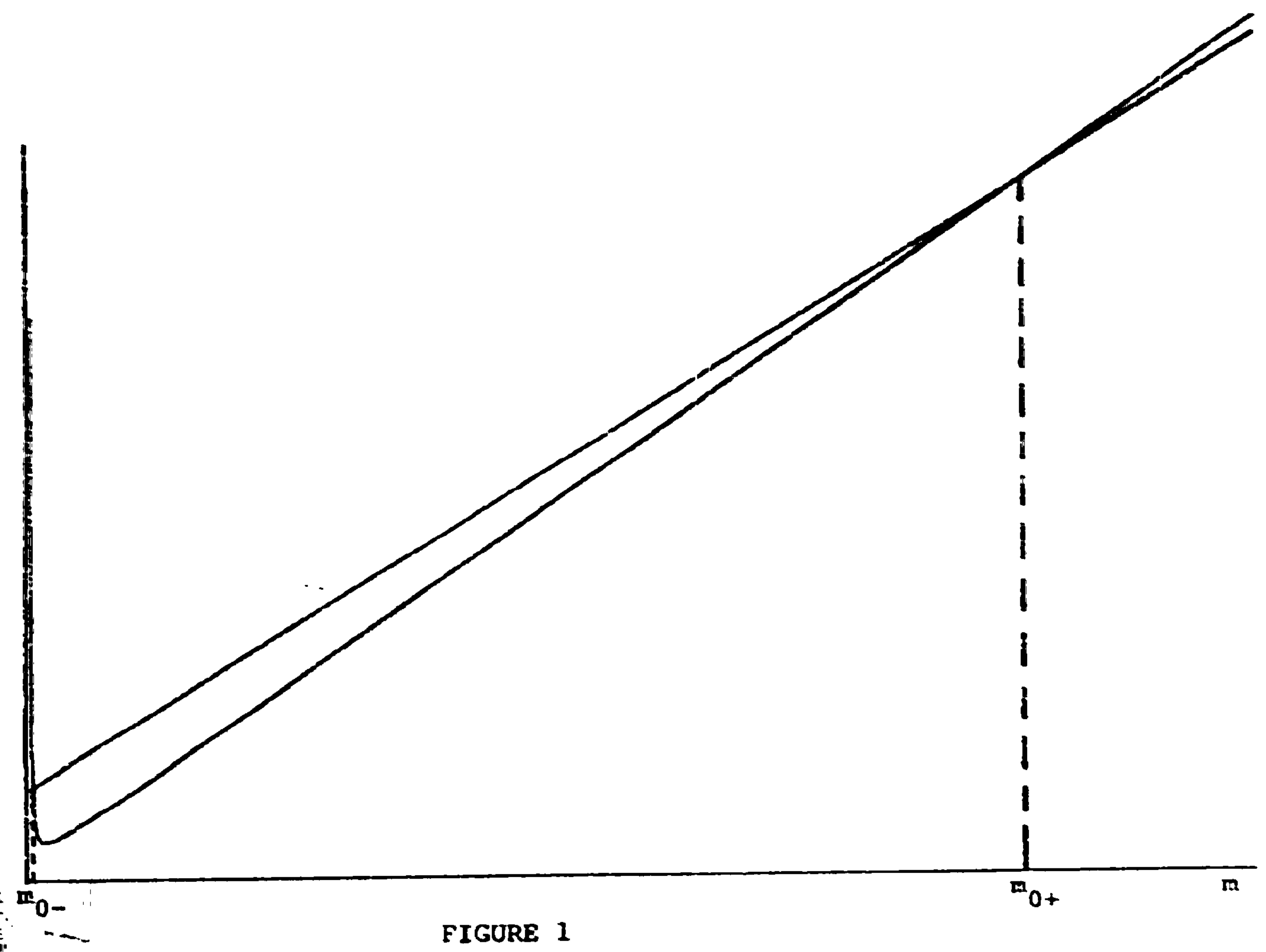


FIGURE 1

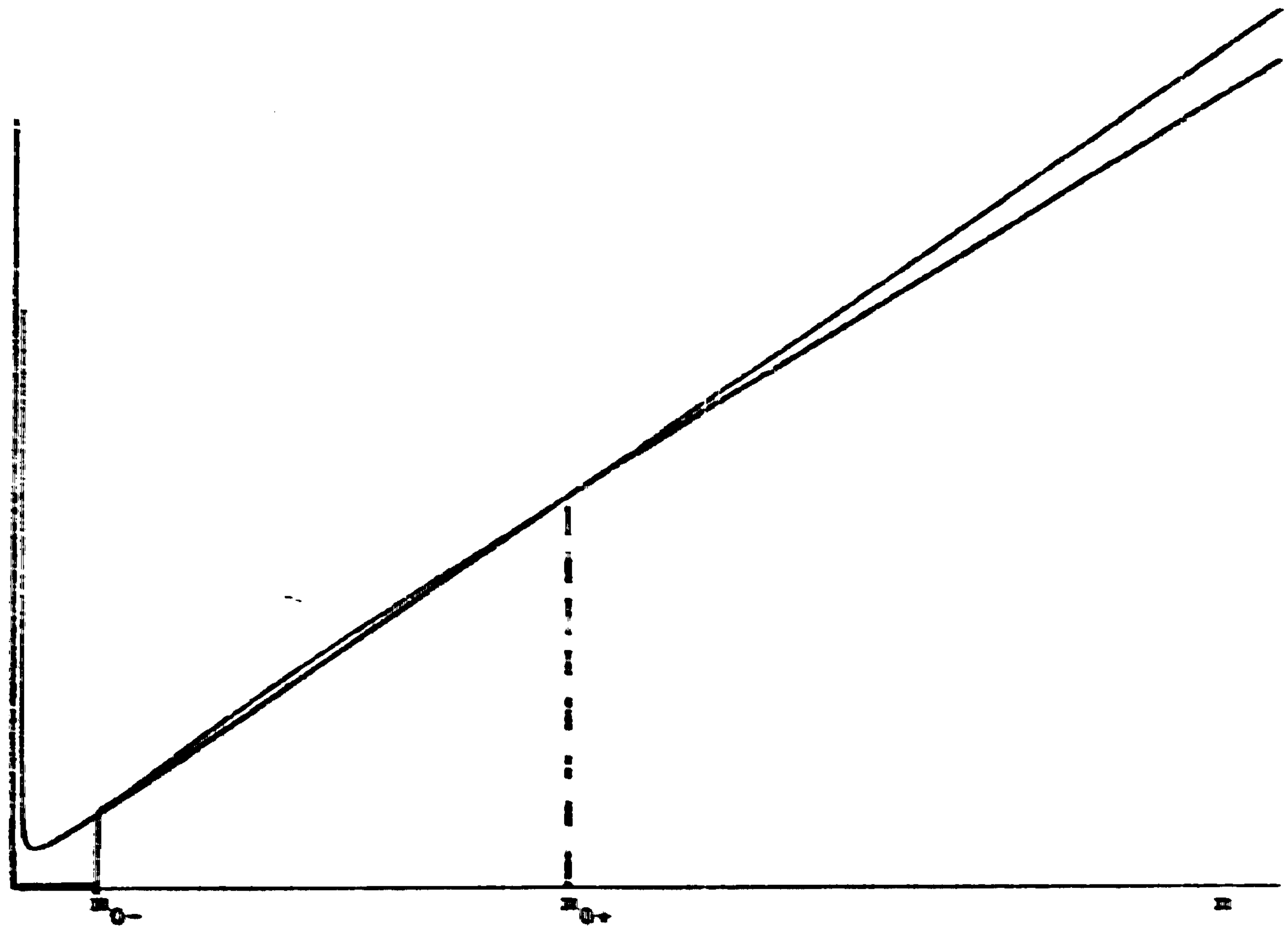
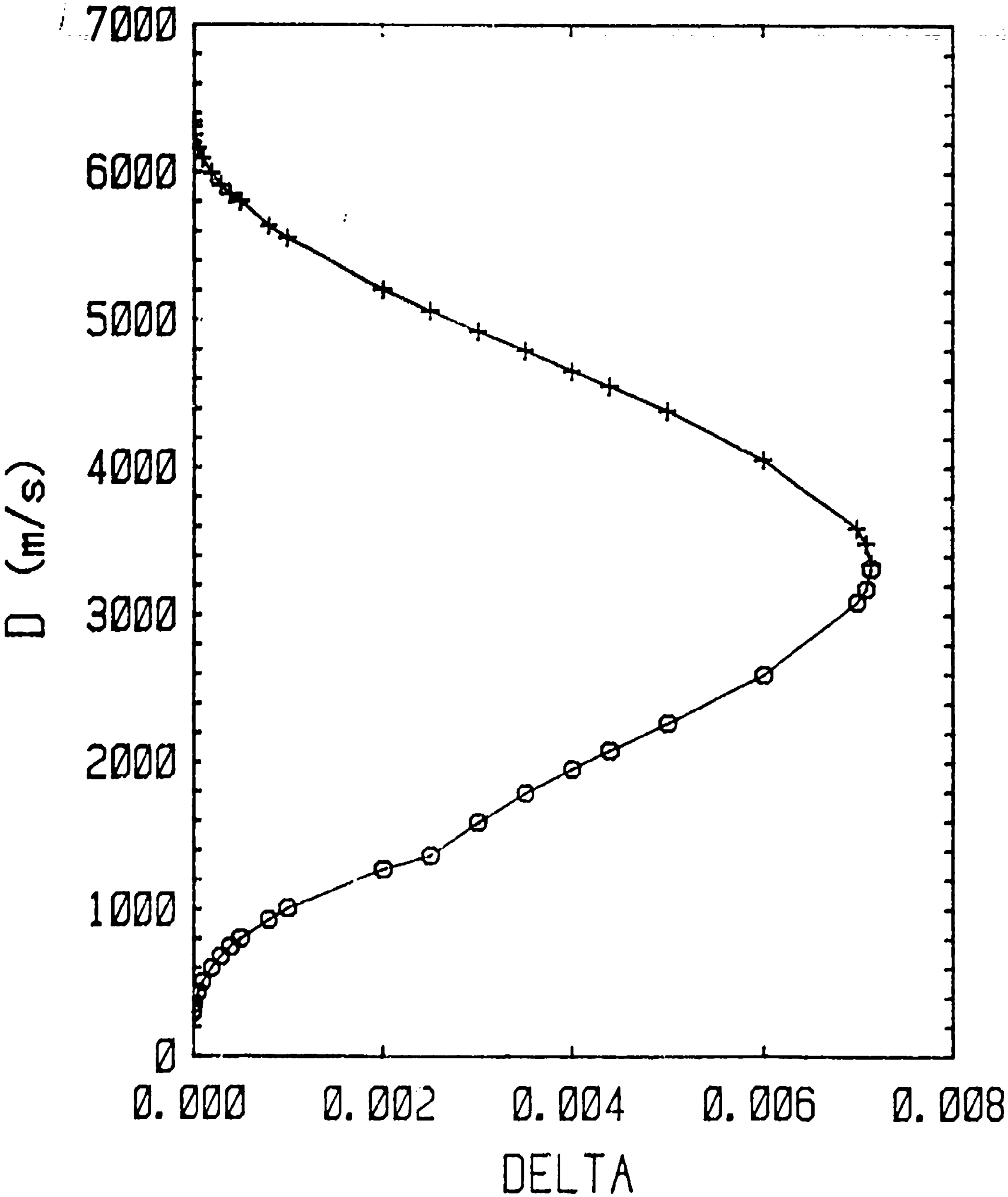


FIGURE 2



7000
6000
5000
4000
3000
2000
1000
0
D (m/s)
0.000
0.002
0.004
0.006
0.008
DELTA

FIGURE 3

University of Miami
Coral Gables, Florida 33124
PHYSICS DEPARTMENT
P.O. Box 248046

December 15,1981

Department of the Air Force
AF Office of Scientific Research
Contracting Officer
Bolling Air Force Base, D.C. 20332

Reference: Minigrant AF AFOSR80-0135, Final Scientific Report.
'Analytical Studies of Non-Ideal Explosives'
P.I. Dr. Manuel A. Huerta
University of Miami, Department of Physics

Attached please find the Final Report for the referenced Minigrant. The Minigrant had a budget of $9,999 and supported 1.75 months of work. The effort was concentrated on obtaining analytical results to describe the variation of the steady detonation velocity with diameter losses. Some interesting results were found.

I would like to express my appreciation for the support I received under this grant.

Sincerely

Manuel A. Huerta

Manuel A. Huerta
Associate Professor of Physics

UNIVERSITY OF MIAMI
CORAL GABLES, FLORIDA 33124

PHYSICS DEPARTMENT
P.O. BOX 248046

MINIGRANT PROPOSAL TO AIR FORCE OFFICE OF SCIENTIFIC RESEARCH

Attention: Major Richard W. Kopka
AFOSR/XOP
Bolling AFB
D.C. 20332

Proposing Institution: University of Miami
Department of Physics
Coral Gables, FL 33124

Title: Analytical Studies of Nonideal Explosives

Budget: $10,000 Proposed Duration: July 1, 1980 - August 31, 1981.

Principal Investigator: Dr. Manuel A. Huerta
Associate Professor of Physics
University of Miami

Manuel A. Huerta

Signature of P.I.
Date: 10/22/'79

G.C. Alexandrakis

Signature of Dr. George C. Alexandrakis
Chairman of the Dept. of Physics
Date: 10/22/79

Signature of Mr. J.A. Burd
Authorized Official
Executive Director of Fiscal Management
Date: ______________

TABLE OF CONTENTS

DESCRIPTION OF PROPOSED RESEARCH

Introduction:

This proposal for a minigrant is a follow-up to the research the P.I. performed at the AFATL at Eglin AFB under the 1979 USAF-SCEEE Summer Faculty Research Program. That research dealt with understanding the behavior of nonideal explosives via their mathematical models. The results of that research are summarized in the Final Report entitled Detonation Physics of Nonideal Explosives With Analytical Results for Detonation Failure Diameter. A copy of that report is attached as the Appendix to this proposal.

The major causes of nonideal behavior discussed in the Appendix are: (i) endothermic and reversible chemical reactions, (ii) heat and lateral expansion losses, and (iii) transverse structure of the front. The first two causes receive some treatment in the Appendix. In the following sections a continuation of the research is proposed.

Detonation Failure:

The study of cause (ii) in the Appendix led to the development of an analytical method that predicts detonation failure diameters and the existence of a "slow detonation" solution of the steady state equations. A number of questions remain to be clarified. First, the P.I. believes that the above solution, which had been found by other authors using numerical schemes, and which really corresponds to a no-shock Chapman-Jouguet deflagration, is an unstable solution under most conditions. In order to demonstrate this it is here proposed to do a stability analysis. The methods developed here will be useful in the work outlined in the next section. Second, the results in the Appendix rest on an iteration scheme whose properties were not fully obtained quantitatively. This was because the equation for the reaction progress variable cannot be integrated in closed form. Under this grant it is proposed to integrate numerically Eqs.(48) and (61) of the Appendix through several iterations to examine the convergence of the iterates toward the solution that is described qualitatively in the Appendix. Since the main features of the solution are already understood, there is good guidance for the success of the numerical methods. The completion of the above plan of work would be a good start to a truly 2 or 3 dimensional treatment of the lateral expansion and the behavior of the gases behind the sonic locus.

Transverse Structure of the Front:

The importance of cause (iii) of nonideal behavior is well established. A good description of recent advances is contained in the book by Fickett and Davis[6]. The development of the Transverse structure is due to the nonlinear growth of instabilities in the 1-dimensional solution. It is here proposed to use the techniques of nonlinear perturbation and bifurcation theory to extend the work of Erpenbeck, cited in Ref. 6, on the formation of transverse front structures.

Connection with Experiment:

Prior to my departure from the HERD laboratory at Eglin AFB, Major James W. Holt, Jr., USAF, Chief of the Explosives Branch at the AFATL, expressed an interest in doing experiments to verify this theory. I will reestablish contact with him to try to arrange this.

Facilities Available:

The numerical calculations will be done on the University of Miami's UNIVAC 1100/81 computer. The budget of the Department of Physics allows the P.I. to have access to large amounts of computer time without charge to this mini-grant.

BUDGET FOR

MINIGRANT PROPOSAL

Manuel A. Huerta
[redacted]

Salaries, Wages and Fringe Benefits

Manuel A. Huerta

Principal Investigator

1980 - 81 Est. Salary $24,200/9 months	
100% time during July 7 - August 15, 1980 (1 1/4 months)	$3361
1981 - 82 Est. salary $26,620/9 months	
100% time during August 3 - August 15, 1981 (1/2 month)	$1479
Fringe Benefits	
14.83% X faculty salary	$ 718
Total of Salaries, Wages and Benefits	$5558

Other Direct Costs

Travel Consists of transportation cost to scientific meetings and visits to other institutions with whom P.I. collaborates on research work pertaining to this proposal.	$ 481
Publication Costs	$ 200
Supplies	$ 50
Total Direct Costs	$6289
Indirect Costs (59% of modified total direct costs)	$3710
TOTAL	$10,000

CURRICULUM VITA

Name: Manuel A. Huerta

Title: Associate Professor of Physics

[redacted]

[redacted]

Professional Experience:

Associate Professor of Physics
University of Miami, Coral Gables, Florida
September 1978

Program Associate (on leave from University of Miami)
U. S. - Latin America Cooperative Science Program
National Science Foundation
May 1977 - August 1978

Associate Professor of Physics
University of Miami, Coral Gables, Florida
May 1975 - (Tenured in May 1976)

Assistant Professor of Physics
University of Miami
September 1972 - May 1975

Associate Research Scientist, Magneto Fluid Dynamics Division
and Adjunct Professor of Mathematics
Courant Institute of Mathematical Sciences, New York University
September 1970 - August 1972

Instructor of Physics
University of Miami
September 1966 - August 1970

Education:

Ph.D. Physics, January 1970: University of Miami, Coral Gables, Florida
Grade Point Average: 4.0
Dissertation: Approach to Equilibrium of Infinite Chains of Coupled Harmonic Oscillators

M. S. Physics, January 1967: University of Miami, Coral Gables, Florida
Grade Point Average: 4.0

B. S. Electrical Engineering, June 1965: California Institute of Technology, Pasadena, California
Grade Point Average: 3.8
Graduated with Honors

Enrolled at University of Miami in Electrical Engineering from September 1961 to August 1963 then transferred to the California Institute of Technology.
Grade Point Average: 3.8

Scholarships:

NASA Fellowship in Physics, University of Miami
September 1965 - August 1966

Graduate Assistant in Physics, Center for Theoretical Studies, University of Miami, Summer of 1965

Undergraduate Scholarship, California Institute of Technology, 1963 - 1965

Undergraduate Scholarship, University of Miami, 1962 - 1963

Honors as Student:

California Institute of Technology's David Joseph McPherson Prize. Awarded upon graduation to the graduating senior in engineering who best exemplified excellence in scholarship.

Membership in Societies:

Tau Beta Pi, Phi Kappa Phi, Sigma Xi, American Physical Society, American Mathematical Society.

Research Fields of Interest:

Plasma Physics, Statistical Mechanics, Solid State Physics, Acoustic Propagation, Nonlinear Partial Differential Equations.

Participation in Research Contracts:

September 1973 - August 1974
P. I. in project entitled "Research in Acoustic Propagation and Reflection from Internal Waves" done under a NOAA Grant No. 04-4-022-9

September 1974 - August 1975
Renewal of above grant

September 1975 - August 1976
Renewal of above grant

August 1979 - July 1980
P. I. in Contract No. AFOSR 78-3663 entitled "The Stability and Dynamics of Elastic Structures and Fluid Flows."

Professional Consulting:

September 1973 - August 1974. Consultant to the Atomic Energy Commission through the Magneto Fluid Dynamics Division of the Courant Institute of Mathematical Sciences of New York University. This work was supervised by Professor Harold Grad, Director of the Division. The consulting agreement was under A.E.C. Contract No. AT(11-1)-3077.

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"Entropy and the Approach to Equilibrium of Infinite Chains of Coupled Harmonic Oscillators", Invited Colloquium, University of South Florida, Tampa, January 1970.

2. "Entropy Oscillations and the H Theorem for Finite Segments of Infinite Coupled Harmonic Oscillator Chains", International Conference on Thermodynamics, Cardiff, Wales, April 1970.

3. "Exact Solutions for Thermal Conductances of Two and Three Dimensional Contacts" 14th International Conference on Thermal Conduction, June 1975, Storrs, Conn.

4. "Secondary Bifurcation Near Multiple Eigenvalues", Meeting of Florida Academy of Sciences, Florida International University, Miami, Florida, March 1979.

Statement of Other Support of Dr. M. Huerta

P.I. in AFOSR Contract No. 78-3663

Title: "The Stability and Dynamics of Elastic Structures and Fluid Flows." This contract supports the study of imperfect bifurcations and secondary bifurcations in elastic structures and fluid flows. It supports 100% of the P.I.'s time during May 15, 1980 - July 6, 1980. The budget for this contract follows.

Revised Budget - AFOSR 78-3663

Salaries and Wages	
Manuel A. Huerta	
Principal Investigator	
1980-81 $24,200/9 months (est.)	
100% time, May 15, 1980 - July 6, 1980	$4705
Fringe Benefits	698
Total Salaries and Fringe Benefits	$5403
Travel Consists of transportation cost to scientific meetings, visits to and visits from scientists at other institutions with whom P.I. actively collaborates on research work pertaining to this proposal	473
Publication Costs	350
Supplies and Communications	110
Total Direct Costs	$6,336
Indirect Costs	
(53% of salaries and benefits)	$2,864
TOTAL	$9,200

1979 USAF - SCEEE SUMMER FACULTY RESEARCH PROGRAM

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FINAL REPORT

DETONATION PHYSICS OF NONIDEAL EXPLOSIVES WITH ANALYTICAL RESULTS FOR DETONATION FAILURE DIAMETER

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DETONATION PHYSICS OF NONIDEAL EXPLOSIVES WITH ANALYTICAL RESULTS FOR DETONATION FAILURE DIAMETER

ABSTRACT

The main causes of nonideal behavior in explosives are examined. An elaboration of the ZND model for 1-dimensional steady detonations is presented as a reference frame from which to examine the effects of reversible chemical reactions endothermic reactions, etc. Mathematical models for 2-dimensional detonations are studied and a preliminary analytical method of solution is presented. The method provides analytical expressions for the detonation failure diameter in terms of the parameters of the detonation. The results obtained help to clarify previous results obtained by other authors using numerical methods. Suggestions for further research are given.

ACKNOWLEDGMENTS

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I. INTRODUCTION

The most powerful high explosive formulations are usually composed of TNT, HMX, RDX and a few other compounds. These substances are relatively expensive and their availability in large quantities is not assured. To head-off a possible shortage of high explosive materials, attempts are being made by the USAF and others to increase the variety of compounds that can be used as high explosive components. Due to its wide availability, ammonium nitrate is one of the most important compounds being incorporated into new high explosive formulations. It is often found that these new formulations do not perform as well as one would expect from their heats of reaction and other thermodynamic data. This deficient performance has led to the use of the term nonideal explosives.

There is no hard definition of nonideal explosives. The situation is similar to that for ideal vs. nonideal gases. A nonideal gas is one whose equation of state differs significantly from the ideal gas law PV=NKT. No real gas is ideal if one looks hard enough, but under the usual conditions of low pressure and high temperature, however, most gases behave very closely to ideal gases. In the case of explosives, ideal behavior is pretty well represented by the Chapman-Jouguet (CJ) theory of detonations. In many cases, where one deals with explosives with fast reaction rates and large diameter charges, there is good agreement between the CJ theory and experiment. In many of the new explosive formulations being developed, however, one finds nonideal behavior. In these nonideal explosives the detonation velocity and pressure are found to be significantly lower than predicted by the CJ theory. This disagreement between theory and experiment has prompted the need for further developments in detonation theory.

The Chapman[1] - Jouguet[2] theory was developed near the turn of the century. There are many good expositions of it such as by Courant and Friedrichs[3] and by Taylor and Tankin[4]. The CJ theory considers the reaction zone to be a discontinuity in a reacting gas, very similar to the usual theory of gas-dynamic shocks. The fluid-flow equations for conservation of mass, momentum and energy are integrated across a 1-dimensional plane detonation discontinuity.

The above is completed with the hypothesis that immediately behind the discontinuity the chemical reactions are completed, and the fluid velocity relative to the discontinuity is sonic. The CJ theory will not be discussed in detail here because more advanced developments are presented below. To compare this theory with experiment one needs the equation of state and the energy equation of the explosive. These equations are not well known for solid explosives. This is typical of the present state of the field, where a lot of important information is just not known. The situation for gases is much better than it is for solids, and satisfactory comparisons between theory and experiment can be made.

The next major step forward in the understanding of detonations took place during World War II with the development of the Zeldovick-Von Neumann[5]-Doering (ZND) theory of detonations. A thorough discussion of this theory as well as many theoretical and experimental aspects of detonations can be found in the recently published book by Fickett and Davis[6]. Von Neumann's rigorous treatment of a 1-dimensional steady detonation wave firms up and clarifies the CJ theory. His discussion of a pathological reaction also introduces a way in which nonideal behavior can occur. His model of a detonation wave is that it consists of a mechanical shock wave that initiates the chemical reaction, followed by a deflagration zone (pressure drops away from shock) where the chemical energy is released.

Present theories for steady detonation waves are extensions of the ZND theory. They include general types of chemical reactions and deviations from 1-dimensional motion. These effects are the main causes of nonideal behavior and will be considered below. This work is organized as follows. Sec II states the research objectives. Sec. III presents a discussion of a fairly general theory of steady detonations. In Sec. IV the theory is specialized to 1-dimensional detonations to highlight the nonideal effects due to various types of chemical reactions. In Sec V the effects of divergent flow are explored. These effects are quite complicated to calculate because the flow is no longer 1-dimensional. This section contains the original results on detonation failure obtained in this research effort. Sec. VI contains the conclusions and recommendations.

II. OBJECTIVES OF THE RESEARCH EFFORT

(1) To survey the present state of detonation theory with a view to obtain a clear understanding of the causes of nonideal behavior in explosives.

(2) To develop analytical methods for obtaining solutions to some of the problems of interest. Specifically, an approximation method is studied that can lead to analytical expressions for calculating the detonation failure diameter of detonating charges.

III. GENERAL DISCUSSION

As the front of a detonation wave passes a point, it leaves behind a gas moving with some velocity. The set of points where the speed of the moving gases relative to the front equals the local speed of sound is called the sonic locus. The strength of the detonation wave depends on the amount of chemical energy that is released between the leading shock front and the sonic locus. Any chemical energy released beyond the sonic locus is lost for the purpose of producing a strong detonation wave although it may still do useful work against confining media. As will be seen below, the CJ theory predicts that in many cases the sonic locus coincides with the point where the chemical reaction is completed so the entire energy released is applied to the detonation wave. Any deviation from this will amount to nonideal behavior. In order to understand the problem one should start with a fairly general model. A good framework is given in the papers of Kirkwood and Wood[7] and Wood and Kirkwood[8]. An even more general starting point is found in Chapters 4 and 5 of Ref. 6. The mathematical model uses the Euler equations for a compressible, nondissipative, reactive medium, undergoing adiabatic motion into which a steady detonation wave is propagating. Let the medium be a cylinder of indefinite length but finite radius. We introduce a system of cylindrical coordinates with Z-axis along the charge axis. The region $Z < 0$ will cover the unreacted explosive. The shock front is at $Z=0$ at $t=0$ and propagates toward $Z < 0$. The region $Z > 0$ covers the zone of reaction. The variables are taken to be independent of the azimuthal angle around the Z-axis.

The equations are:

$$\dot{\rho} + \rho\left(\frac{\partial u}{\partial z} + \frac{\partial \omega}{\partial r}\right) + \rho\frac{\omega}{r} = 0 \quad , \qquad (1)$$

$$\rho\dot{u} + \frac{\partial p}{\partial z} = 0 \quad , \qquad (2)$$

$$\rho\dot{\omega} + \frac{\partial p}{\partial r} = 0 \quad , \qquad (3)$$

$$\dot{E} - \frac{p\dot{\rho}}{\rho^2} = 0 \quad , \qquad (4)$$

and $$\dot{\lambda}_i = R_i = F_i(1-\lambda_i) \quad , \quad i = 1, \ldots, j. \qquad (5)$$

Here ρ is the mass density; u and ω are the mass velocity components in the Z and r directions respectively; p is the fluid pressure; E is the internal energy per unit mass; and the λ_i are a set of reaction progress variables for the j chemical reactions taking place with the reaction rates R_i. An equation of state $E = E(p, \rho, \lambda_i)$ is assumed known. A form often used is

$$E(p, \rho, \lambda_i) = \frac{p}{\rho(\gamma - 1)} - \sum_{i=1}^{j} \lambda_i q_i \qquad (6)$$

where the q_i are the heats per unit mass released in the reactions. The dot (.) notation means that the connective derivative is taken

$$\cdot \equiv \frac{\partial}{\partial t} + u\frac{\partial}{\partial z} + \omega\frac{\partial}{\partial r} \qquad (7)$$

We will just consider a steady detonation wave located at $Z=0$. The unreacted fluid rushes in from the left with a detonation speed D (to be determined). We also specialize the equations to the Z axis where $r=0$ and $\omega=0$. The result is

$$u \frac{\partial \rho}{\partial z} + \rho \frac{\partial u}{\partial z} = -2\rho \frac{\partial w}{\partial r} \quad , \quad (8)$$

$$\rho u \frac{\partial u}{\partial z} + \frac{\partial p}{\partial z} = 0 \quad , \quad (9)$$

$$\frac{\partial p}{\partial r} = 0 \quad , \quad (10)$$

$$\frac{\partial E}{\partial z} - \frac{p}{\rho^2} \frac{\partial \rho}{\partial z} = 0 \quad , \quad (11)$$

and

$$u \frac{\partial \lambda_i}{\partial z} = R_i \quad , \quad i = 1, \ldots, j. \quad (12)$$

The Von Neumann model is to assume that for $Z < 0$ the flow quantities are constant with values ρ_0, p_0, $D = u_0$, $\lambda_1 = 0$. At $Z = 0$ there is a mechanical shock with jumps to ρ_1, p_1, u_1 but still $\lambda_1 = 0$. For $Z > 0$ the reactions develop accompanied by changes in ρ, p, and u. The Mach numbers

$$M_0 = \frac{D}{c_0} \quad , \quad (13)$$

Where c_0 is the sound speed in front of the shock, and

$$M_1 = \frac{D}{c_1} \quad , \quad (14)$$

Where c_1 is the sound spped right behind the shock, are related by

$$M_1^2 = \frac{2 + (\gamma - 1) M_0^2}{2\gamma M_0^2 - (\gamma - 1)} \quad , \quad (15)$$

in accordance with the usual shock relations

$$\frac{p_1}{p_0} = \frac{2\gamma M_0^2 - (\gamma - 1)}{\gamma + 1} = q \quad , \quad (16)$$

and

$$\frac{\rho_1}{\rho_0} = \frac{(\gamma + 1) M_0^2}{2 + (\gamma - 1) M_0^2} \quad , \quad (17)$$

as found in Landau and Lifshitz[9]. A solution of the shock conditions with no discontinuity, so $p_1 = p_0$, $\rho_1 = \rho_0$, and $M_1 = M_0$, is also allowed. Eq. (8) - (11) can be integrated with the boundary conditions at $Z=0^+$ and $Z=0^-$

$$\rho(0^+) = \rho_1 \ , \quad p(0^+) = p_1 \ , \quad u(0^+) = u_1 \qquad ,$$

$$\rho(0^-) = \rho_0 \ , \quad p(0^-) = p_0 \ , \quad u(0^-) = D \qquad , \quad (18)$$

to yield

$$\rho_0 D = \rho_1 u_1 = \rho u + 2\rho_0 D I_2 \qquad , \quad (19)$$

$$\rho_0 D^2 + p_0 = \rho_1 u_1^2 + p_1 = \rho u^2 + p + 2\rho_0 D^2 I_3 \qquad , \quad (20)$$

and

$$H_0 + \tfrac{1}{2} D^2 = H_1 + \tfrac{1}{2} u_1^2 = H + \tfrac{1}{2} u^2 \qquad , \quad (21)$$

where H is the enthalpy per unit mass,

$$H = E + p/\rho \qquad , \quad (22)$$

and

$$I_2 = \frac{1}{\rho_0 D} \int_0^z \rho \frac{\partial \omega}{\partial r} dz \qquad , \quad (23)$$

and

$$I_3 = \frac{1}{\rho_0 D^2} \int_0^z \rho u \frac{\partial \omega}{\partial r} dz \qquad , \quad (24)$$

in the notation of Chapter 5 of Ref. 6. The integrals I_2 and I_3 represent losses due to the radially divergent flow. In one dimensional flow they would be zero. Bernoulli's equation along the axis, Eq. (21), is not affected by the radial flow. The important equation

$$\frac{\partial u}{\partial z} = \frac{\sum_i \sigma_i R_i - 2\,\partial\omega/\partial r}{1 - u^2/c^2} \qquad , \quad (25)$$

can be obtained from Eqs.(8)-(12). The σ_i are given by

$$\sigma_i = \frac{1}{\rho c^2} \left(\frac{\partial p}{\partial \lambda_i}\right)_{E,\rho,\lambda_j} \qquad , \quad (26)$$

with

$$c^2 = \frac{1}{\rho^2} \frac{(p - \rho^2 \partial E/\partial \rho)}{\partial E/\partial p} = \left(\frac{\partial p}{\partial \rho}\right)_{S,\lambda} \qquad . \quad (27)$$

The above equations can describe the steady flow region. Eq. (25) has a singularity at $u=c$, the sonic locus. Beyond this point the flow has to match the boundary conditions at Z large. Generally the flow beyond the sonic locus is some sort of time dependent rarefaction wave. Fig. 1 is a diagram of the situation.

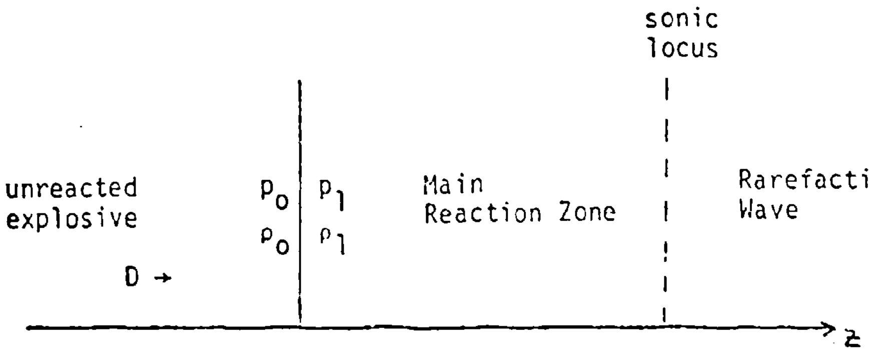

Fig. 1. Main regions of a detonation wave seen in the frame of the shock front.

The equations in this section allow for a fairly realistic and mathematically very complicated model. In Sec. IV we specialize the equations to the much simple 1-dimensional flow where $\omega=0$. In Sec. V we consider some aspects of 2-dimensional flows.

IV. 1-DIMENSIONAL THEORY

Putting $\omega=0$ and $\partial/\partial r=0$ in the equations of Sec. III we obtain a 1-dimensional theory. The results of this section are standard and are presented to fix the notation and nomenclature that is needed in Sec. V. Eliminating u from Eq. (19) and (20) one obtains

$$p-p_0=\rho_0^2 D^2\left(1/\rho_0 - 1/\rho\right) \quad .(28)$$

In a p vs. $1/\rho$ plot, the graph of Eq. (28) is a straight line called the Rayleigh line. Eliminating u and D from Eq. (21) one obtains

$$E(p,\rho,\lambda_i)-E(p_0,\rho_0,0)=\tfrac{1}{2}(p+p_0)\left(1/\rho_0 - 1/\rho\right), \quad (29)$$

which is a family (as one varies λ_i) of curves, in a p vs. $1/\rho$ plot, known as Hugoniot curves. As we move in Z behind the front, the λ_i are related because from Eq. (12) we have

$$\frac{d\lambda_1}{R_1}=\frac{d\lambda_2}{R_2}=\cdots\cdots=\frac{d\lambda_j}{R_j} \quad . \quad (30)$$

Thus in effect a single λ parametrizes the Hugoniot family. So far D is not determined so the slope of the Rayleigh line $(-\rho_0^2 D^2)$ is unknown. Yet the intersection of the Rayleigh line with the Hugoniot curves will determine the solution. The answer is obtained by noting that Eq. (25) gives a singularity for $\partial u/\partial z$ at the sonic locus unless we have

$$\sum_{i=1}^{j}\sigma_i R_i = 0 \quad . \quad (31)$$

(we are in 1-dimension, so $\omega=0$). Eq. (31) must be imposed at the sonic locus to avoid the singularity for the reasons given in Chapter 5 of Ref. 6. Eq. (31) determines the value of the λ_i and thus picks a particular Hugoniot curve, at the sonic locus. Noting that $u=c$ at the sonic locus, and using Eq. (19), we have that the slope of the Rayleigh line is

$$-\rho_o^2 D^2 = -\rho^2 c^2 \quad . \quad (32)$$

We also have that the slope of the Hugoniot curves is

$$\left.\frac{\partial p}{\partial(1/\rho)}\right|_{\mathcal{H}} = -\frac{\left[\frac{1}{2}(p+p_o) - \rho^2 \partial E/\partial\rho\right]}{\left[\partial E/\partial\rho - \frac{1}{2}(1/\rho_o - 1/\rho)\right]} \quad . \quad (33)$$

Combining Eqs. (27), (32), and (33), we get for the slope of the Hugoniot curves

$$\left.\frac{\partial p}{\partial(1/\rho)}\right|_{\mathcal{H}} = -\rho^2 c^2 \quad . \quad (34)$$

Thus, the slope of the Rayleigh line is the same as the slope of the Hugoniot curve (which is determined by Eq. (31)) at the sonic locus. For the case where there is only one reaction Eq. (31) becomes R=0 or λ=1 at the sonic locus. This means that the one reaction is completed at the sonic locus. This justifies the CJ hypothesis which determines the Rayleigh line (and thus D) by putting it tangent to the completed reaction Hugoniot. For the equation of state of Eq. (5), the above method yields that D satisfies

$$D^4 - 2D^2 c_o^2\left[1 + \frac{\lambda q(\gamma^2-1)}{c_o^2}\right] + c_o^4 = 0 \quad . \quad (35)$$

Eq. (35) has the two roots

$$D_\pm^2 = c_o^2 M_{o\pm}^2 = c_o^2\left\{1 + \lambda q\frac{(\gamma^2-1)}{c_o^2} \pm \sqrt{\left[1 + \lambda q\frac{(\gamma^2-1)}{c_o^2}\right]^2 - 1}\right\} \quad . \quad (36)$$

The two roots give two Rayleigh lines called R+ and R-. R+ represents a CJ detonation while D- represents a CJ deflagration. These are depicted in Fig. 2. For the CJ- solution the solution goes smoothly along R- from to the values at CJ- attained at the sonic locus. No shock takes place for this deflagration solution. For the detonation, the Von Neumann model is that the solution goes along the no reaction Hugoniot from O to N, $p=p_1$ and $\rho=\rho_1$ (with p_1 and ρ_1 determined from Eqs. (16) and (17) using Eq (36) for M_o) and then down from N to CJ+ along R+. A detonation solution going directly from

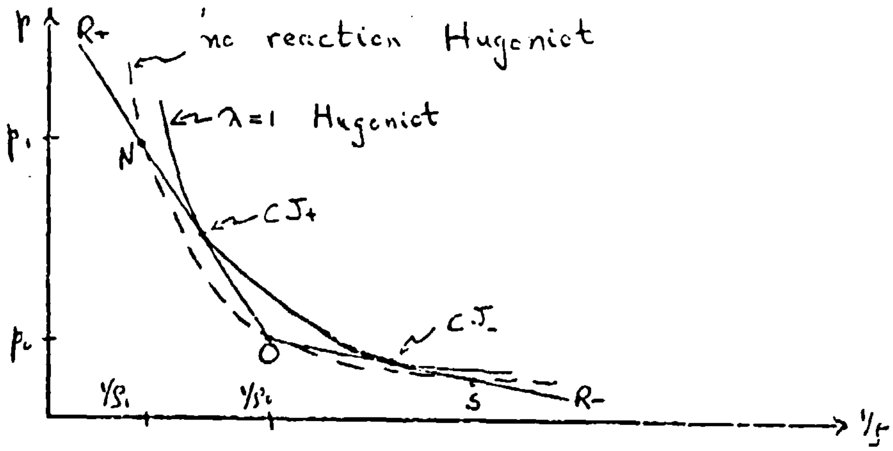

Fig. 2. The p- $^1/\rho$ plane. CJ+ gives the pressure at the sonic locus for a detonation. CJ- gives the pressure for a deflagration

O to CJ+ along R+ with no shock is also allowed. Both solutions have the same final state CJ+ at the sonic locus and the same D. The no shock solution does not usually occur because of problems with initiating the reaction. The Von Neumann model in fact says that the O→CJ+ detonation is actually a mechanical shock to p_1 followed by a deflagration from N to CJ+. Due to the way that the equations integrate through a shock, the point CJ+ is the same with or without a Von Neumann spike.

The CJ hypothesis is that the sonic locus is determined by tangency of the Rayleigh line to the completed reaction Hugoniot. If there are several irreversible exothermic reactions this hypothesis is correct (for 1-dimensional, steady flows). If some of the reactions are reversible, however, or if some of the σ_i may be negative as in mole decrement reactions, then Eq. (31) does not imply that the reactions are completed at the sonic locus.

Thus some of the chemical energy is released beyond it. This late energy is not effective in the detonation and nonideal behavior is found. The analysis of precisely what happens involves a study of the phase plane of Eq. (25). Many complicated results are possible depending on the details of the σ_i and the R_i. A fairly thorough discussion of the possibilities can be found in chapter 5 of Ref. 6, and in Wood and Salsburg[13].

This brief discussion of steady, 1-dimensional detonations does not cover the entire subject. In this research effort we have made no contribution to this part of the field. There are good analytical methods, that supplemented by computer calculations, can predict the nonideal performance of steady, 1-dimensional detonations. An input to these methods, however, must contain a realistic description of the reaction kinetics. This is presently not known for most gaseous explosives, let alone solid ones. In the case of solid explosives, beyond the lack of information concerning the equation of state and the reaction kinetics, there are also the problems associated with inhomogeneous mixtures. Here the effects due to grain burning and diffusion of reactants are not fully worked out.

V. DIVERGENT FLOW AND DETONATION FAILURE

When ω is not negligible, Eqs. (8)-(12) need to be complemented by a way to compute $\frac{\partial \omega}{\partial r}$ as a function of Z. This depends on the shape of the exploding charge and on the properties of the confining media. In general, to compute ω one must solve a difficult free boundary problem with matching at the boundary to account for the properties of the different media. Even if ω were known, however, there are still some interesting difficulties in integrating Eqs. (8)-(12). These equations should predict the observed phenomenon of detonation failure when the diameter of the exploding cylinder is small. We will cast those equations in the form for flow in a nozzle by letting

$$\frac{1}{A}\frac{dA}{dz} = \frac{2}{u}\frac{\partial \omega}{\partial r} \quad , \qquad (37)$$

where A is the area of the nozzle. The equations become

$$\frac{d}{dz}(\rho u A) = 0 \quad . \qquad (38)$$

$$\frac{du}{dz} = \frac{\sum_{i=1}^{j} \sigma_i R_i - \frac{u}{A}\frac{dA}{dz}}{1 - u^2/c^2} \quad . \qquad (39)$$

$$\frac{d\lambda_i}{dz} = R_i/u \quad , \qquad (40)$$

and

$$\frac{d}{dz}\left(H + u^2/2\right) = 0 \quad . \qquad (41)$$

Several authors have taken the above equations with realistic rate terms and applied computer methods to obtain a variety of results. Some of this work is summarized in Chapter 5 of Ref. 6. Wecken" takes

$$\frac{1}{A}\frac{dA}{dz} = \epsilon = \text{constant} \quad , \qquad (42)$$

with one Arrhenius reaction to discuss the structure of the reaction zone. He is not successful in obtaining detonation failure at some critical ϵ because of computational difficulties. Tsuge et al.[12] take

$$\frac{dA}{dz} = \frac{1}{\sigma_1}\left[\frac{P g - A}{(1 + \delta k M_0^2)A - P g}\right]^{1/2} \quad , \qquad (43)$$

where σ_1 is the value of the thickness σ of an explosive slab at Z = 0, g is given in Eq. (16),

$$A = \frac{\sigma}{\sigma_1} \quad , \quad P = \frac{p}{p_1}A \quad , \quad \text{and} \quad k = \frac{\rho_{01}}{\rho_0} \quad , \qquad (44)$$

where ρ_{00} is the density of the confining medium. Eq. (43) is obtained by treating the lateral expansion as a blunt body about which the confining inert flows. Tsuge et al. take a very detailed description of the reaction kinetics for $H_2 + \frac{1}{2} O_2 \rightarrow H_2O$ and solve the problem numerically. Their comparisons with experiment for exploding slabs are fairly good. Their numerical calculations lead to plots as shown in Fig. 3. For $\sigma_1 < \sigma_c$ there is no detonation solution, so detonation failure is found in this model. For $\sigma_1 > \sigma_c$ they obtain two solution branches. The upper branch is like the usual 1-dimensional detonation M_{0+} of Eq. (36). They did not explore the lower branch fully because of computational difficulties. They speculate that as $\sigma_1 \rightarrow \infty$ the lower branch has $M_0 \rightarrow 1$. It will be shown here that this is incorrect. The limit of the lower branch as $\sigma_1 \rightarrow \infty$ is actually $M_0 \rightarrow M_{0-}$ as in Eq. (36).

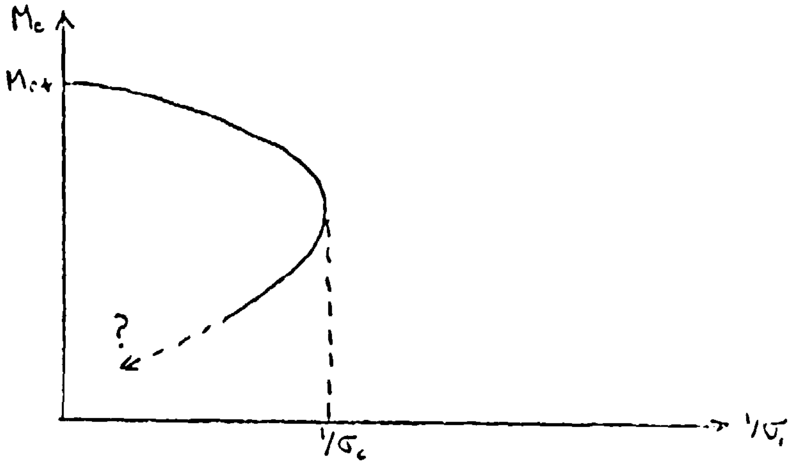

Fig. 3. Rough plot of Mo vs. $1/\sigma$ in Tsuge et al.[12]

Rather than attacking this problem numerically from the beginning we will try to develop the solution analytically as far as possible. We use the equation of state given in Eq. (6). Then the σ_i defined in Eq. (26) (not to be confused with the σ and σ_1 above which were lengths) are given by

$$\sigma_i = \frac{(\gamma-1)}{c^2} q_i \quad , \quad (45)$$

where

$$c^2 = \frac{\gamma p}{\rho} = \frac{2(\gamma-1)}{2+(\gamma-1)M^2}\left[\sum_i \lambda_i q_i + H + u_1^2/2\right] . \quad (46)$$

We rewrite Eq. (39) as

$$\frac{2(1-m)}{m(1+\gamma m)[2+(\gamma-1)m]}\frac{dm}{dz} = \frac{\frac{d}{dz}\sum_i \lambda_i q_i}{\sum_i \lambda_i q_i + H_i + u_i^2/2} - \frac{2}{1+\gamma m}\frac{1}{A}\frac{dA}{dz} ,$$

where $m = M^2 = u^2/c^2$. (47)

Eq. (47) is to be solved so that dm/dz remains finite at m=1. A necessary condition for this is that the right hand side of Eq. (47) be zero when m=1. Also at Z=0, λ=0 and $m=m_1$ with m_1 to be determined. These are unusual boundary conditions to impose on a first order ordinary differential equation. Eq. (47) does not satisfy the usual Lipschitz condition needed for the existence of a solution with a desired value of m at a specific Z . But the unusual boundary conditions are sufficiently "free" that a solution will exist. We do not fix the Z where m=1 occurs, the sonic point Z, but we let the equation tell us so as to keep dm/dz finite. Then we find the value m_1 . Since the problem presented by Eq. (47) is not a standard one it is unclear that a Picard iteration method will converge for it. We have found useful results with this method, so we will use it with the awareness that it may need modification due to convergence difficulties. The n^{th} iteration of m, m^n will be found from

$$\frac{2(1-m^n)}{m^n(1+\gamma m^n)[2+(\gamma-1)m^n]}\frac{dm^n}{dz} = \frac{\frac{d}{dz}\sum_i \lambda_i^n q_i}{\sum_i \lambda_i^n q_i + H_i^n + u_i^{n2}/2} - \frac{2}{1+\gamma m^{n-1}}\frac{1}{A}\frac{dA}{dz} , \quad (48)$$

where n = 2,3,....

with the right hand side of Eq. (48) equal to zero when $m^n = 1$. We also need to use Eq. (40). The first iterate m^1 is found by putting the dA/dz term equal to zero. The equation for m^1 can be integrated to get

$$\frac{m'[2+(\gamma-1)m'][1+\gamma m_1']^2}{(1+\gamma m')^2 \; m_1' \; [2+(\gamma-1)m_1']} = \frac{\sum_i \lambda_i q_i + \frac{c_1^2}{2(\gamma-1)}[2+(\gamma-1)m_1']}{\frac{c_1^2}{2(\gamma-1)}[2+(\gamma-1)m_1']} \; , \quad (49)$$

where $$m_1' = m'(z=0) \; , \quad (50)$$

and where we have used Eq. (46) evaluated at $Z=0$, with $c_1 = c(Z=0)$. Imposing the right hand side condition for the m equation we get

$$\frac{d}{dz}\sum_{i=1}^{j} \lambda_i q_i = 0 \quad \text{at} \quad m' = 1 \; . \quad (51)$$

If all the q_i are positive, and the R_i are as given in Eq. (5), we need that for the first iteration, at the sonic point Z_s^1,

$$m'(z_s') = 1 \quad , \quad \lambda_i(z_s') = 1 \; . \quad (52)$$

For the simple R_i this implies $Z_s^1 = \infty$. We go to Eq. (49) and put $\lambda_i = 1$ when $m^1 = 1$ to find m_1^1. The result is that m_1^1 obeys the equation

$$\frac{(1+\gamma)(1+\gamma m_1')}{(1+\gamma)^2 \quad m_1'} = [2+(\gamma-1)m_1'] + \frac{2(\gamma-1)}{c_1^2}\sum_i q_i \; . \quad (53)$$

Manipulating this equation yields

$$(m_1')^2 - 2m_1'\left[1 + \frac{(\gamma^2-1)}{c_1^2}\sum_i q_i\right] + 1 = 0 \; . \quad (54)$$

Eq. (54) is almost the same as Eq. (35). The difference is that in Eq. (35) we have c_0 and $D = M_0 c_0$ whereas c_1 appears in Eq. (54). If we consider the case with no shock, then $c_1 = c_0$, $m_1^1 = m_0^1$, and we have the same result as in Eq. (35). The solutions obtained would refer to a no-shock detonation that goes along 0-CJ+ and a no-shock deflagration that goes along 0-CJ-. The second of these is meaningful, but not the first. If we consider the case with a shock we put

$$c_1^2 = \frac{\gamma p_1}{\rho_1} = \frac{\gamma p_0}{\rho_0} \frac{\left[2\gamma m_0^1 - (\gamma-1)\right]\left[2 + (\gamma-1) m_0^1\right]}{(\gamma+1)^2 \, m_0^1} \tag{55}$$

into Eq. (54) to get, after using Eq. (15),

$$(m_0^1)^2 - 2 m_0^1 \left[1 \quad \frac{\gamma^2 - 1}{c_0^2} \sum_i q_i \right] + 1 = 0 \quad . \tag{56}$$

This is exactly the same as Eq. (35), just as it should be because the R+ line in Fig. 2 is the same whether we consider a shock solution along 0-N-CJ_+, or a no shock one along 0-CJ_+. The two solutions of Eq. (56) are interpreted as a Von Neumann detonation along 0-N-CJ_+, and an unphysical shocked deflagration along 0-S-CJ- . Out of the four solutions obtained we only desire the shocked detonation 0-N-CJ_+, and the no-shock deflagration 0-CJ- . Their detonation velocities are given by the roots $D_+ = c_0 M_{0+}$ and $D_- = c_0 M_{0-}$ of Eq. (35). Using Eq. (15) we get the m_{1+}^1 that goes with M_{0+} while the m_1^1 that goes with M_{0-} is $m_{1-}^1 = M_{0-}$ . . Knowing m_{1+}^1 and m_{1-}^1 we go to Eq. (49) and we get m_+^1 and m_-^1 as functions of $\lambda_1(z)$. Finally from Eq. (40) we can integrate to get $\lambda^1(z)$. This first iterate reproduces the results of Sec. IV because dA/dz was neglected. But we begin to see the source of the two roots in the work of Tsuge et al.[12] When we compute the next iteration the results of the expansion will come in. But as the diameter goes to ∞ the expansion becomes negligible and the results reduce to m_+^1 and m_-^1 . To compute m^2 we go to Eq. (48) with n=2. We integrate it with the boundary condition

$$m^2(z=0) = m_1^2 \quad . \quad (57)$$

The result is

$$\ln\left\{\frac{m^2[2+(\gamma-1)m^2](1+\gamma m_1^2)^2}{(1+\gamma m^2)^2 m_1^2[2+(\gamma-1)m_1^2]}\right\} = \ln\left\{\frac{\sum \lambda_i^2 q_i + H_1^2 + (u_1^2)^2/2}{H_1^2 + (u_1^2)/2}\right\} - 2\int_0^z \frac{1}{1+\gamma m^2}\frac{1}{A}\frac{dA}{dz}dz \quad .$$

(58)

m_1^2 is determined by imposing the bounded dm^2/dz condition to the right hand side of Eq. (48) with n=2. At the sonic point Z_s^2 we have

$$\frac{1}{\sum_i \lambda_i^2 q_i + H_1^2 + (u_1^2)^2/2} \sum_i q_i \frac{(1-\lambda_i^2)F_i}{c}\bigg|_{z_s^2} = \frac{1}{1+\gamma m^2}\frac{1}{A}\frac{dA}{dz}\bigg|_{z_s^2} \quad . \quad (59)$$

Eq. (40) was used to obtain Eq. (59). The latter equation says that $\lambda_1 \neq 1$ at the sonic point so the reactions are not completed. Some of the energy will be released late leading to nonideal behavior. In principle Eq. (59) determines Z_s^2 in terms of m_1^2 . This can be seen as follows. We have that

$$\frac{(c)^2}{\gamma-1} + \frac{(u)^2}{2}\bigg|_{z_1^2} = H_1 + \frac{(u_1)^2}{2} = \frac{(c)^2}{\gamma-1} + \frac{(c)^2}{2}\bigg|_{z_s^2} \quad , \quad (60)$$

so that c in Eq. (59) is known in terms of m_1^2 and c_1 . Also from Eq. (40)

$$\frac{d\lambda_i^2}{dz} = \frac{R_i}{m^2 c} \quad . \quad (61)$$

In Eq. (61) m^2 is known in terms of λ^2 from Eq.(58). (We assume that $\frac{1}{A}$ dA/dz is explicitly known as a function of Z). Therefore one can integrate Eq. (61) to get λ^2 as a function of Z and m_1^2. When this function $\lambda^2(Z, m_1^2)$ is substituted into Eq. (59) one can find Z_s^2 as a function of m_1^2 as claimed. Now we go back to Eq.(58) and demand that

$$m^2(z_s^2) = 1 , \quad \lambda_i^2(z_s^2) = \lambda_i^2(z, m_1^2) \equiv \lambda_{is} , \quad (62)$$

and get

$$\frac{(1+\gamma m_1^2)^2}{(1+\gamma)\, m_1^2} = 2+(\gamma-1)m_1^2 + \frac{2(\gamma-1)}{(C_1)^2}\sum_i \lambda_s q_i - 2\left[2+(\gamma-1)m_1^2\right]\int_0^{z_s^2} \frac{1}{1+\gamma m'}\,\frac{1}{A}\frac{dA}{dz}\,dz . \quad (63)$$

In Eq. (63) Z_s^2 and λ_s^2 are functions of m_1^2. So Eq. (63) is an equation for m_1^2. The last terms is the expansion dependent term. Let

$$\Delta(\epsilon) = 2\int_0^{z_s^2} \frac{1}{1+\gamma m'}\,\frac{1}{A}\frac{dA}{dz}\,dz . \quad (64)$$

Here ε represents an inverse diameter that goes to zero as the diameter goes to ∞. Also $\Delta(\varepsilon) \to 0$ as $\varepsilon \to 0$ or as the expansion is negligible. Eq. (63) is rewritten as

$$(m_1^2)^2\left[1+(\gamma^2-1)\Delta\right] - 2m_1^2\left[1+\frac{\gamma^2-1}{(C_1)^2}\sum_i \lambda_{is} q_i - \Delta(1+\gamma)\right] + 1 = 0 . \quad (65)$$

This equation reduces to Eq. (54) as $\Delta \to 0$ and $\lambda_s^2 \to 1$ as $\varepsilon \to 0$. Thus there is a clear connection between the two branches to be obtained from Eq. (65) and thel-dimensional results. The two roots of Eq. (65) are obtained by the quadratic formula as

$$m_1^2 = \frac{\left[1+\frac{(\gamma^2-1)}{(C_1)^2}\sum_i \lambda_{is} q_i - \Delta(1+\gamma)\right] \pm \sqrt{\left[1+\frac{(\gamma^2-1)}{(C_1)^2}\sum \lambda_{is} q_i - \Delta(1+\gamma)\right]^2 - \left[1+\Delta(\gamma^2-1)\right]}}{\left[1+\Delta(\gamma^2-1)\right]} . \quad (66)$$

For small ε these two roots give the m_+^1 and m_-^1 of before which were connected with the m_{0+}^1 and m_{0-}^1 of Eq.(35). As ε and Δ grow beyond a critical value the two roots become complex, so there is no real solution and detonation failure takes place. To simplify things let us ignore the variation of λ_s^2 with ε . Then a plot of the roots versus Δ appears as in Fig. 4. This is qualitatively the same as the curve

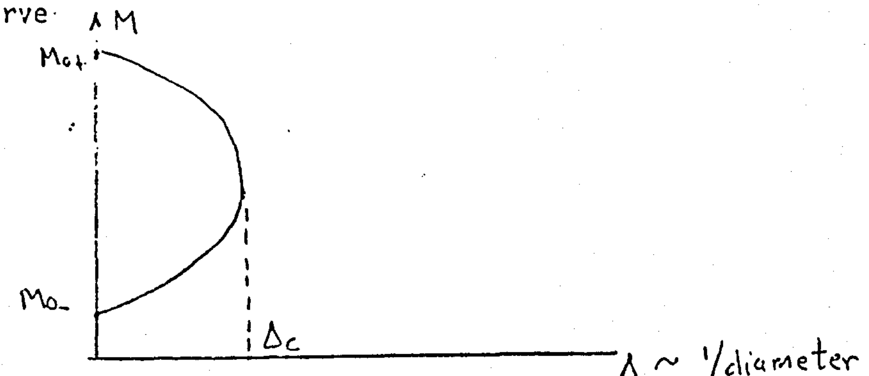

Fig. 4. Plot of M_0 vs. 1/diameter.

obtained numerically by Tsuge et al. For $\Delta < \Delta_c$ (for the diameter greater than some critical value) there are two branches. The upper branch is connected as $\Delta \to 0$ to the 1-dimensional shocked detonation 0-N-CJ_+ of Fig. 2. The lower branch is connected as $\Delta \to 0$ to the 1-dimensional no-shock deflagration 0-CJ_- .Now one sees the error in the work Tsuge et al. They could compute things like Z_s^2 and λ_s^2 numerically but with so much difficulty that the results were hard to interpret.

The qualitative features of the solution are now clear. To get quantitative results one needs to integrate Eq. (61). This would have to be done numerically. It is clear that successive steps in the iteration are not very different from the steps to calculate m^2 . No theoretical problems with convergence should arise although this should be checked numerically in some specific examples. We propose to do this in future work. The critical value Δ at which detonation failure occurs is given by

$$1 + (\gamma^2 - 1)\Delta_c \geq \left[1 + \frac{\gamma^2-1}{(C_1)^2} \sum_i \lambda_{is} q_i - (1+\gamma)\Delta\right]^2 \quad . \qquad (67)$$

It would be interesting to explore ways in which this behavior could be checked with experiment. It should be noted that this theory predicts that the speed of deflagrations increases as the diameter decreases. At some critical diameter the detonation and deflagration velocities are the same and for smaller diameters there is no solution.

VI CONCLUSIONS AND RECOMMENDATIONS

The causes of nonideal behavior can be summarized in three categories.

(i) Incompletely effective use of the chemical energy for the detonation wave due to the nature of the chemical reactions. If there are reversible or endothermic reactions, the effects ar especially important. For steady 1-dimensional flows the physical theory is prepared to handle the problem. The knowledg of the burning rates of the relevant chemical reactions, however needs to be improved.

(ii) Loss of strength due to the lateral expansion of the explosive. Here the state of the physical theory is not so good. In Sec. V we presented a calculation for detonation failure. The radial flow was not calculated but was assumed known. The analytical solution presented should be checked with numerical calculations A further step would be to compare these results with experiment The author would like to be able to pursue these further developments.

(iii) Loss of strength due to transverse structure of the front and non-steady phenomena in the detonation. These effects are interesting per se and their effects on nonideal behavior are judged to be important[6]. These wave instability problems were not addressed in this research effort because the author felt he needed a good understanding of the simpler aspects of nonideal behavior before addressing them. There is much room for research into these effects using the techniques of nonlinear stability analysis and bifurcation theory.